MST e NEWS

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After a successful academic career, Laurent Capolungo recently returned to Los Alamos to perform innovative materials research. Shown here in front of a screen projection of materials modeling code, he retains his affection for teaching, often helping younger scientists develop their computational mechanics skills. Photo credit Michael Pierce, XIT-TSS

Laurent Capolungo

"MST-8 is one of the top groups in materials science and metallurgy ... I knew coming back to Los Alamos would be a chance to do impactful research."

Returning to the Lab to create materials solutions

By Kris Fronzak, ADEPS Communications

As Laurent Capolungo watched tons of molten metal pour out of a vat in a fiery sheet, radiating heat, he had a revelation. Then an intern at a European steel manufacturer, Capolungo (Materials Engineering in Radiations and Dynamics Extremes, MST-8), decided to focus his career on materials. This "a-ha moment" has guided him since; materials are always at its heart.

Capolungo, who was a postdoctoral researcher at Los Alamos, recently returned as a scientist on MST-8's Dynamic and Quasi-Static Loading Modeling Team. The opportunity to perform groundbreaking materials science with top-notch colleagues lured him away from a tenured associate professorship at Georgia Institute of Technology.

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“To have more direct communication with all employees in MST Division, I will be periodically coming around to your team meetings where we can discuss important issues on your mind, such as research/ program direction, management concerns, safety/security issues, career opportunities etc., or you can use the opportunity to share some recent research progress.”

From David’s desk . . .

We are in a period of transition: the presidential administration change, the LANL M&O contract change, and a significant renewal of our workforce through a hiring campaign. Periods of change or transition can create significant uncertainty and also increase our anxieties about our future. One way I can help you all through this change is to increase my level of communication with you and help you understand what these changes might mean. With a new administration, we will likely see changes in programmatic priorities and direction. In the President’s FY18 Budget submission, we certainly saw some indications of a higher priority on our nuclear weapons mission and less emphasis on applied energy programs. However, the House and particularly the Senate budget proposals restored much of the applied energy and basic science budgets while still investing strongly in our nuclear weapons program. In MST Division, we have not yet seen any negative effects of this national debate. In fact, our overall budgets have increased and our FY18 budget projection looks solid. As many of you are aware, the LANS contract will expire in October 2018 and a new contractor will begin managing the Laboratory after that. The final Request for Proposals (RFP) was issued on October 25, 2017 and proposals are due by December 11, 2017—less than a month away. The M&O contract change should not directly affect your day-to-day work. We will likely see a change in senior management, which may change high-level structure or organization, but you should not see a significant change in the type of work you are doing or the programs on which you are working. I’ll keep you updated as we learn more about the contract change. If you have questions, please ask me or check the Lab’s RFP FAQ page. Lastly, to prepare for the anticipated attrition rates and ensure we are able to successfully deliver on mission requirements, MST Division has been hiring quite a few new employees, both internally and externally. A particular challenge with bringing in such a large, new workforce is training, mentoring, and helping them become accustomed to the Lab. MST will launch an MST Workforce Development Initiative in the new year that will include expectations for managers, team leaders, mentors, and workers to develop career development plans and to identify mentor opportunities. The Lab has had a focus on this with postdocs and early-career scientists, however, we will be expanding this approach to include all employees in MST Division.

An initiative that I am leading for ADEPS is the Employee Engagement Initiative that resulted from the LANL-wide employee survey. Two focus areas were identified for this initiative: improved communication and first-line manager training. As we look for ways to improve our communication across ADEPS, I would appreciate hearing ideas from you on how we can improve this communication. Sometimes, we as managers think we are communicating what we believe is important; however, there may be other issues on your mind that you would like to hear more about. To have more direct communication with all employees in MST Division, I will be periodically coming around to your team meetings where we can discuss important issues on your mind, such as research/program direction, management concerns, safety/security issues, career opportunities etc., or you can use the opportunity to share some recent research progress.

Lastly, as we enter the holiday season, we can become distracted and possibly stressed with family obligations or meeting end-of-the-year deliverables. Before performing work, please remember to “take 5” to reaffirm that you understand that your work fits within approved work scope and authorization and that you understand the procedures for performing the work safely. A “take 5” should be something we routinely do, but becomes especially important when we may have higher than normal distractions or stress. Also, keep an eye out for your fellow co-workers and help them perform their work safely, securely, and compliantly.

Thanks for another great year!

MST Division Leader David Teter

Capolungo cont.

“I worked very hard for years to get tenure, but once I got it I realized I didn’t want to risk settling,” Capolungo said. “MST-8 is one of the top groups in materials science and metallurgy, and I knew coming back to Los Alamos would be a chance to do impactful research.”

Since returning he has launched into research, developing and validating mathematical models for materials applications. Key to his work is the concept of co-design, where theory informs experiments, which in turn improve simulations, in a potentially endless co-design loop.

“I came to Los Alamos as a hardcore modeler, but my mentor, Carlos [Tomé], opened my eyes to how much richness comes from integrating experiments with modeling,” he said.

“Laurent acts upon his ideas, familiarizes himself with the available literature, and then creates from that point,” said Tomé (MST-8). “In the course of his short career he has become an expert on a panoply of research subjects and made original contributions to most of them, some of which will guide future research efforts.”

To date his most complex project has been applying code that he developed to predict a metallic material’s performance and its microstructure evolution during irradiation and the force of mechanical loading. Capolungo’s three-dimensional discrete dislocation dynamics (DDD) code is being used to develop a new mesoscale material model that simulates plasticity in polycrystalline metals. DDD will help researchers understand the effects of defect interactions on materials performance. The Los Alamos Laboratory-Directed Research and Development project will also assess the potential use of both acoustic and diffraction signatures to nondestructively quantify microstructure state with improved accuracy.

“By combining experiments with a computational component, we will develop a new model that extracts much more information than we ever could before,” said team member Ricardo Lebensohn (Fluid Dynamics and Solid Mechanics, T-3).

Capolungo, who has PhDs in micromechanics from France’s Paul Verlaine University and from Georgia Tech, has improved the interpretation of diffraction peaks, which determine the crystal structure of materials. His use of discrete dislocation methods has informed constitutive models of plasticity used in material design.

He retains his affection for teaching, working with MST-8 students and new hires to develop their computational mechanics skills. Capolungo also collaborates with universities to bring students to Los Alamos and develops capabilities benefitting their schools and the Lab.

“Every subject attracts his attention and he rapidly develops insights about it and recognizes the relevant aspects of the problem,” said Tomé. “Laurent has an incredible capability to produce and work.”

Laurent Capolungo’s favorite experiment

What: Measure the three-dimensional elastic strain tensor in the neighborhood of a twin in deformed magnesium.

Why: The experiments conducted at the Advanced Photon Source could largely improve our understanding of diffusionless transformations in hexagonal close-packed metals by providing data that can be used to validate/invalidate our conceptualization of twinning.

Who: Arul Kumar (lead), Carlos Tomé, Bjorn Clausen, Rod McCabe (MST-8)

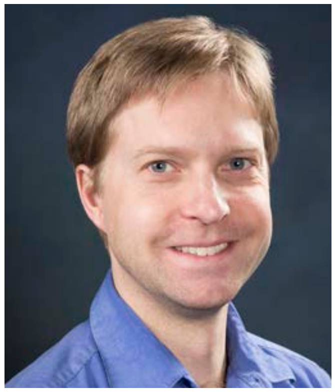
When: 2016

Where: Advanced Photon Source at Argonne National Laboratory

How: We leveraged the experience gained within our Office of Basic Energy Sciences program over more than a decade and studied the literature to propose a novel yet feasible experiment. We teamed up with Advanced Photon Source scientists from the preparation phase all the way to the data interpretation phase.

MST staff in the news

Beaux receives 'best pitch' award at DisrupTECH



For his plan to bring internet access to remote places using floating Wi-Fi hotspots, Miles Beaux (Engineered Materials, MST-7) was granted the "best pitch" award among Los Alamos staff scientists at the Lab's third annual DisrupTECH event. His patent-pending technology uses ultra-low-density solid materials to create pseudo-weather balloons that float without gas and could be affordably deployed in hard-to-reach places.

Beaux, who has a PhD in physics from the University of Idaho, conducts actinide research using photoemission spectroscopy and scanning probe microscopy. He is an expert in thin and thick film deposition and materials synthesis and characterizations of one-dimensional nanomaterials. A former Seaborg Postdoctoral Fellow, he received a Los Alamos Awards Program team award in 2014 and an individual award in 2016. He was the principal investigator of a 2017 Institute for Materials Science Rapid Response grant and holds two patents.

DisrupTECH brought together investors, business leaders, and others to learn about potentially disruptive technologies—those that could potentially change the way we live and work—being developed at the Lab. Five Los Alamos staff scientists and 6 postdoctoral researchers pitched different technologies to a panel of industry experts and venture investors.

Other MST researchers pitching ideas at the event were

- Brenden W. Wiggins (MST-7), who proposed using barium-incorporating glass sensors as a low-cost method of gamma ray detection, and
- Markus Hehlen (MST-7), who proposed integrated technology that would provide first responders with information in real-time, revolutionizing situational awareness in emergencies.

The event was hosted by Los Alamos's Richard P. Feynman Center for Innovation, the New Mexico Angels investor group, and the New Mexico Start-Up Factory. Sponsors included title sponsor EY, the State of New Mexico Economic Development Department, the New Mexico Manufacturing Extension Partnership, the Los Alamos Commerce and Development Corporation, the County of Los Alamos, and the City of Albuquerque.

Technical contact: Miles Beaux

Parker receives Distinguished Student Performance Award

Scott Parker (Engineered Materials, MST-7) received a 2017 Los Alamos Distinguished Student Performance Award. The annual awards, sponsored by the Student Programs Advisory Committee and the Student Program Office, recognize outstanding performance by Lab students.

Parker was nominated by Andy Nelson (MST-7) for his work on a Los Alamos Laboratory-Directed Research and Development (LDRD) Mission Foundations project on the electrolytic reduction of plutonium surrogate oxides. Parker was responsible for the characterization portion of the project, which is expected to expand the Lab's capabilities in plutonium science. He delivered a full report on the research, providing analysis that helped the LDRD team decide which alternative surrogates to investigate and identified possible future issues.

Parker began his graduate research at Los Alamos in 2013, studying high temperature steam oxidation kinetics of candidate cladding materials. He completed his master's degree at University of California, Berkeley and continued graduate research with the Lab's ceramic fuels research group. His PhD thesis is on the manufacture and characterization of thorium and uranium nitride composites.

Technical contact: Scott Parker

Wilson, Takajo win outstanding materials science poster awards at Lab's 2017 Student Symposium

Tashiema Wilson (Engineered Materials, MST-7) and Shigehiro Takajo (Materials Science in Radiation and Dynamics Extremes, MST-8) won outstanding poster awards at the 17th Annual Student Symposium. Wilson's research was on uranium silicide and uranium-silicide-nitride (U-Si-N) and Takajo analyzed microstructural analysis of deformed stainless steel.

Their posters were two of more than 200 presentations at the event, which allows LANL students to present their research and to network and make professional contacts. Organized by the National Security Education Center Student Programs Office, this year's symposium, "Championing Scientific Careers," was held at the University of New Mexico–Los Alamos.

Wilson, who is working toward a PhD in nuclear engineering at the University of South Carolina, Colombia, is mentored

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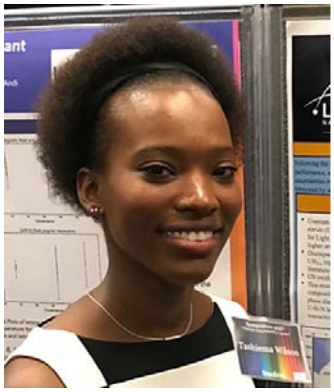
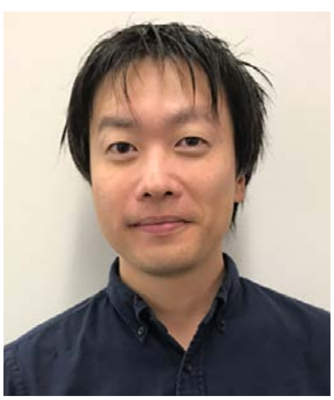
MST staff cont.



by Joshua White (MST-7) and Elizabeth Wood (formerly MST-7, now University of Texas at San Antonio).

Her poster was on experimental analysis of selected uranium silicide and uranium-silicide-nitride." The 2011 Fukushima-Daiichi nuclear disaster prompted the DOE to begin funding research into improving the safety, reliability, and economy of nuclear fuel systems through the consideration of alternative fuel and cladding concepts. These accident-tolerant fuel concepts seek to also improve performance, and therefore focus on materials with higher uranium densities when compared to the traditional (UO_2), such as binary uranium-silicides and uranium silicide-uranium nitride composite fuel forms. These materials have been studied in the past, but recent experimental findings show that uncertainties remain about their fundamental behavior. Wilson studied four compositions between U_3Si_5 and USi_2 that were fabricated by arc melting depleted U with elemental Si. Additionally, in an effort to understand the UN-U_3Si_2 fuel system, an unidentified U-Si-N ternary was observed in samples fabricated by arc melting U_3Si_2 in the presence of varied concentrations of N_2 in argon. Wilson's research also included the preparation and analyses of five compositions including structural characterization using x-ray diffraction and compositional analysis. Her work, which supports the Lab's Energy Security mission and its Materials for the Future science pillar, was funded by the DOE Office of Nuclear Energy's Nuclear Energy University Programs and Advanced Fuels Campaign.



Takajo, who will pursue his PhD in material science at Ibaraki University in Japan, is mentored by Sven Vogel (MST-8).

He presented research on microstructure analysis of gas gun deformed 304L stainless steel. He and his colleagues characterized a 304L stainless steel cylindrical projectile produced by additive manufacturing. The projectile was compressively deformed using a gas gun, causing a significant strain gradient along the sample axis. Spatially resolved neutron diffraction measurements on HIPPO, the high-pressure-preferred orientation diffractometer, and SMARTS, the spectrometer for materials research at temperature and stress, with Rietveld and single peak analysis were used to quantitatively evaluate volume fractions of α, γ, and ε phases and residual strain and texture. The texture of the γ phase is consistent with uniaxial compression while the α texture can be explained with a Kurdjumov-Sachs relationship from the γ texture after deformation, indicating that the material first deformed in the γ phase and subsequently transformed at larger strains. The ε phase was only found in volumes close to the undeformed material with a texture connected to the γ texture by the Shoji-Nishiyama orientation relationship. Takajo concluded that the ε phase occurs as an intermediate phase at lower strain, superseded by the α phase when the strain is further increased. The study showed a proportionality between the root-mean-squared microstrain of the γ phase, dominated by dislocation density, with the α volume fraction, consistent with the strain induced martensite α formation. With knowledge of the sample volume with the ε phase from the neutron diffraction, the team identified the ε phase on the grain level using electron backscatter diffraction, complementing the neutron diffraction analysis. Takajo's work, which supports the Lab's Energy Security mission and the Materials for the Future science pillar, was funded by JFE Steel Corporation.

Technical contacts: Tashiema Wilson and Shigehiro Takajo

Gray inducted to National Academy of Engineering

Rusty Gray (Materials Science in Radiation and Dynamics Extremes, MST-8) is inducted into the National Academy of Engineering by NAE Chairman Gordon England (left) and President Dan Mote (right) for contributions to understanding the dynamic and shock-loading deformation and damage response of materials. The induction was held at the NAE's Annual Meeting in Washington, D.C. Election to the academy is among the highest distinctions an engineer can attain.

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MST staff cont.

MST Division staff recognized for distinguished performance

Five members of MST Division received large team 2016 Los Alamos National Laboratory Distinguished Performance Awards, acknowledging their outstanding contributions to the Laboratory's programmatic efforts.

Above, the pRad Experimental 0631 Team. Below, the PF-4 Readiness Team.

PF-4 Readiness Team

In 2016, the PF-4 Readiness Team, which includes Jay Matthew Jackson of Nuclear Materials Science (MST-16), completed the last three processes to restart programmatic operations at the Lab's Plutonium Facility (PF-4), following DOE requirements for restarting Hazard Category 2 nuclear facilities. Operations in the facility ceased in June 2013.

The team took on restart activities for the pyrochemical process operations; the furnace, casting, and ARIES operations; and the aqueous chloride and americium operations. These operations jointly comprise 28 pieces of equipment that support high-priority missions such as nuclear material purification for pit manufacturing, directed stockpile work, and work for DOE's Office of Science.

Members were required to recreate the technical baseline for all the operations—this was the largest set of readiness activities ever undertaken at Los Alamos. Team members had to identify, retrieve, or create the documentation associated with installation, safety basis, criticality safety, maintenance, and procurement. They also had to adopt new procedures and new training regimes and rigorously implement Conduct of Operations.

Restart activities for each of the three groups of operations lasted 9 to 12 months and were subject to three levels of scrutiny from assessors at the institutional, contractor, and federal level. The team ultimately achieved readiness ahead of schedule while establishing process improvements to benefit all future readiness activities at the Laboratory and across the entire DOE complex. Thanks to the team's work, programmatic operations are being executed at PF-4, and Los Alamos was recognized as a "Center of Excellence" for readiness in 2016.

Other team participants were from Actinide Process Support (MET-1), Pit Integrated Technologies (MET-2), Defense and Space Power Systems (MET-5), Weapon Component Manufacturing and Surveillance (NCO-1), Actinide Process Chemistry (NCO-2), Pit Disposition & Precision Fabrication (NCO-4), Nuclear Component Operations Support Services (NCO-6), Actinide Analytical Chemistry (C-AAC), Inorganic Isotope and Actinide Chemistry (C-IIAC), Deployed ESH at TA-55 (DESHF-TA55), Heavy/Equip Roads and Grounds Operations Craft Resources (LOG-HERG), Plutonium Strategy Infrastructure (PSI), TA-55 Facility Operations Division Office (TA-55-DO), Plutonium Science and Manufacturing (ADPSM), Fire Protection Division Office (FP-DO).

The pRad Experimental 0631 Team

The Proton Radiography (pRad) Experimental 0631 Team brought a weapons-related experiment from concept to completion in less than three months. The idea for Experiment 0631 emerged from a Lab-wide meeting of Weapons Program participants, which addressed the need for experimental data to solve a substantial issue of interest to the program. The idea resulted in a call for an experiment at the Los Alamos Neutron Science Center pRad facility.

The experiment team, which included Engineered Materials (MST-7) members Tana Cardenas, Franklin Fierro, John Martinez, and Derek Schmidt, faced difficult challenges. These included a tight beam schedule and the availability of facilities workers responsible for all aspects for preparation

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MST staff cont.

—from manufacturing and procuring parts, machining conventional and high explosives, completing the experimental assembly, deploying diagnostics, and executing a proof shot checking the design's safety.

Team members were ready to execute the experiment on February 20, 2016—the last possible date available to them. The experiment provided the Lab's Weapons Program with a unique dataset in an unpredicted area that will be further explored. It also resulted in efforts to restore small-scale plutonium experiments at the pRad facility, and serves as a reminder of what Los Alamos can accomplish in the face of unprecedented challenges.

Other team participants were from Applied Modern Physics (P-21), Neutron Science and Technology (P-23), Plasma Physics (P-24), Subatomic Physics (P-25), Focused Experiments (J-3), HE Machining and P&T (J-8), Experiments Integration Office (J-EI), Shock and Detonation Physics (M-9), Weapons Facilities (WFO-WF), XTD Primary Physics (XTD-PRI), and Institutional Systems Services (XIT-ISS).

Isolating microstructural effects on observed strength of additively manufactured stainless steel

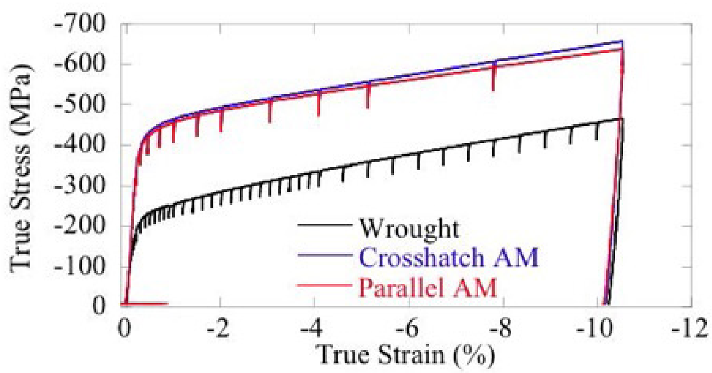
Recent measurements taken at SMARTS, the spectrometer for materials research at temperature and stress, provide a better understanding of how different additively manufactured (AM) microstructural features can be controlled to produce predictable properties.

The quasi-static mechanical strength of AM materials often exceeds that of traditionally wrought counterparts. The AM process results in a distinct microstructure in 304L steel, including unique grain morphology, high dislocation density, and ferrite content—all of which affect the strength. Through precise measurements, researchers can provide a recipe to design microstructure-aware process models that enable science-based qualification of AM components.

In situ heat treatment measurements completed on SMARTS, a technology located at the Lujan Neutron Scattering Center that uses neutron diffraction to probe metals and structural materials, showed that the dislocation density decreases at 700 °C, while the ferrite persists until 950 °C. Electron backscatter diffraction completed at Sandia National Laboratories (SNL) showed that the unique grain morphology persists until ~1200 °C. Five samples were created by tailored heat treatments to eliminate individual portions of the microstructure.

In 2017 in situ deformation measurements will be completed to isolate the effect of each microstructural feature on the strength of the material, boosting understanding of the relationship between process, structure, and properties. The measurements will show how different microstructural features associated with AM can be controlled to produce predictable properties, in support of the Laboratory's vision of controlled functionality in materials.

SMARTS, the spectrometer for materials research at temperature and stress, is located at the Lujan Neutron Scattering Center at the Los Alamos Neutron Science Center.



The graph depicts observed strength differential between additively manufactured and wrought material.

The Lujan Center at the Los Alamos Neutron Science Center provides unique hardware and software capabilities for rapid bulk microstructural characterization to accelerate qualification of AM materials. These results are an example of decades of experience with large datasets that provide the foundation for data analysis of MaRIE experiments in material discovery. MaRIE is the Laboratory's proposed experimental capability for studying matter-radiation interactions in extremes.

The research was funded by the C1 and C2 Science Campaigns (LANL program managers Ray Tolar and Dana Dattelbaum, respectively). Material provided by Sandia National Laboratories. Researchers include Reeju Pokharel, Bjorn Clausen, and Don Brown (Materials Science in Radiation and Dynamics Extremes, MST-8); and Dave Adams and Paul Specht (SNL). Reference: submitted to *Metallurgical and Materials Transactions A*.

Technical contact: Don Brown

Using density functional theory to examine defects in unalloyed δ-plutonium

Understanding the aging of face-centered cubic (fcc) delta (δ)-phase plutonium (Pu) stabilized with gallium is a key issue in stockpile stewardship, as questions of the effects of plutonium self-irradiation on phase stability remain unanswered. To further understand self-irradiation-induced defect formations, Los Alamos researchers conducted a comprehensive study of various classical point defects that include gallium (Ga, an alloying impurity) and uranium (U, a radioactive daughter decay product) in unalloyed δ-plutonium. The journal *Scripta Materialia* published their findings.

In many metals, self-irradiation causes damaging effects in the lattice while inducing void swelling, but aged plutonium does not void swell like other fcc alloys, such as austenitic steel. The mechanisms that inhibit void swelling in plutonium have not been fully investigated, and the fundamental physical role of gallium during radiation damage is unclear. Increasing the gallium concentration has been shown to increase or have no influence on the relative lattice swelling. Although experimental results can provide insight into plutonium aging, first principles and molecular dynamics may guide research into the existence of certain point defects in the lattice that are induced from radiation damage, such as vacancies, interstitials, and <100> split-interstitials.

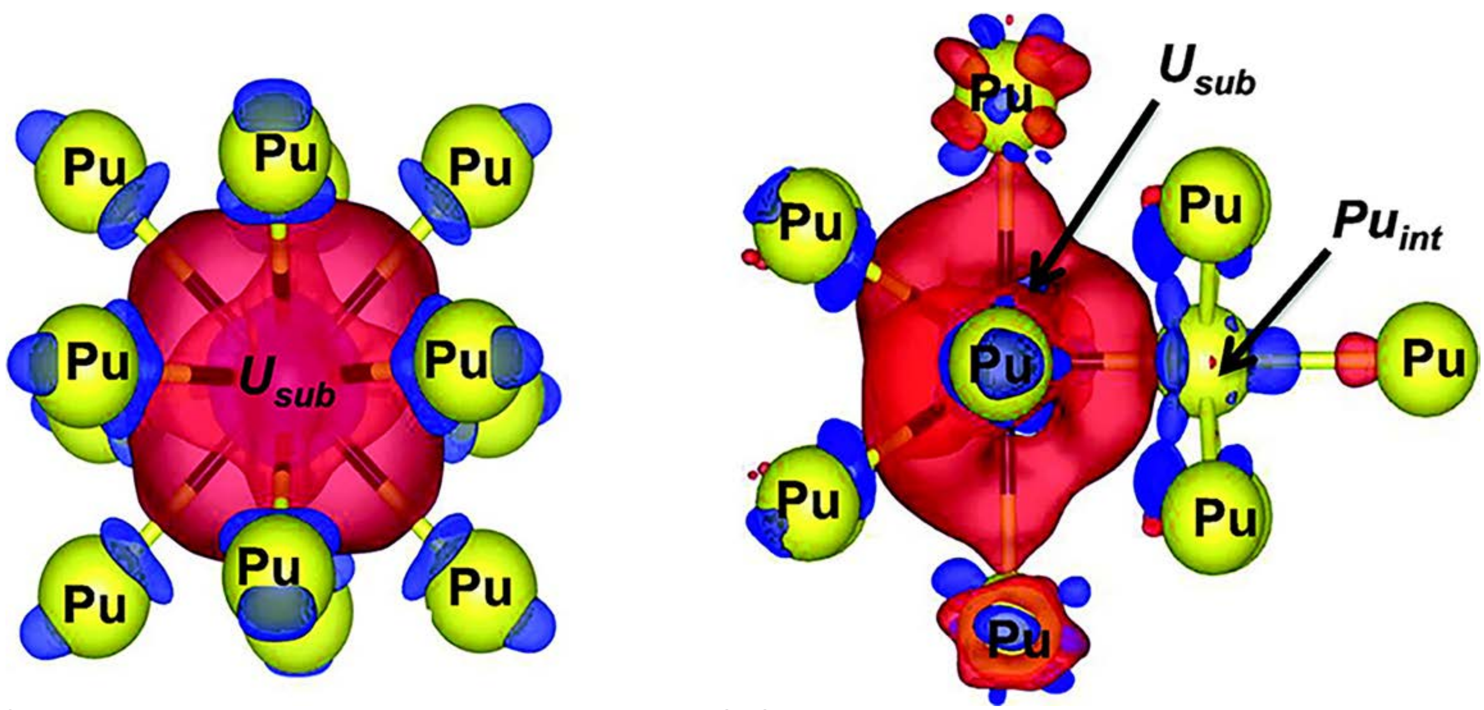
Density functional theory (DFT), a modeling method for simulating material properties, is a useful technique to study the influence of these point defects on the geometric and electronic properties of unalloyed δ-plutonium. Classification of defects by energetics calculated by DFT could identify possible candidates of defects in unalloyed δ-plutonium that affect the structural stability.

The researchers determined that for plutonium-only defects, the most energetically stable defect is a distorted split-interstitial. Gallium, the δ-phase stabilizer, is thermodynamically stable as a substitutional defect, but becomes unstable when participating in a complex defect configuration. Complex uranium defects may thermodynamically exist as uranium substitutional with neighboring plutonium interstitial. Stabilization of uranium within the lattice is shown via partial density of states and charge density difference plots to be 5f hybridization between uranium and plutonium.

Reference: "Density Functional Theory Study of Defects in Unalloyed δ-Pu," *Scripta Materialia* **134**, 57 (2017). Authors: Sarah C. Hernandez and Franz J. Freibert (Nuclear Materials Science, MST-16), and John M. Wills (Physics and Chemistry of Materials, T-1).

The Laboratory Directed Research and Development program funded the work, and Laboratory Institutional Computing provided computational support. The research benefitted from Los Alamos's expertise and capabilities in actinide science research and computing, including the High Performance Computing platforms on the Open Collaborative Network. The research supports the Laboratory's Nuclear Deterrence mission and the Materials for the Future science pillar.

Technical contact: Sarah Hernandez



Charge density difference distribution of uranium substitutional (left) and of uranium substitutional with nearby plutonium interstitial (right) in *fcc* lattice. Red regions indicate charge accumulation, while blue regions indicate charge depletion.

MST's inaugural university outreach workshop fosters research opportunities

The Materials Science and Technology (MST) Division recently hosted a two-day University Outreach Workshop on Nuclear Materials in Los Alamos's Materials Science Laboratory.

The event, organized by Kimberly A. DeFriend Obrey (Materials Science in Radiation and Dynamics Extremes, MST-8), brought together Laboratory staff and professors from seven universities to discuss research opportunities and collaborations. It was the first in a planned series of workshops designed to form collaborations with key professors by having their students intern at the Lab early in their graduate career. The workshops also provided an opportunity for professors to join the Lab as guest scientists or through sabbatical appointments.

Presentations by experts in the field highlighted recent research, novel techniques, and unique capabilities. Speakers included the following.

- Mechanical property evaluations on irradiated materials on multiple length scales—Peter Hosemann (University of California, Berkeley)
- Taming the plasma-material interface under reactor-relevant magnetic fusion condition—Jean Paul Allain (University of Illinois Urbana, Champaign)
- Microstructural evolution in nuclear materials and fuel—Maria Okuniewski (Purdue University)
- Investigating radiation effects in materials by neutron total scattering—Maik Lang (University of Tennessee, Knoxville)
- Development of radiation tolerant ferritic steels for fast reactor applications—Stu Maloy (MST-8)
- Development of high density fuels for light water reactors—Andy Nelson (Engineered Materials, MST-7)
- Atomistic modeling of nuclear materials, a survey—Blas Uberuaga (MST-8)
- Crystallographic modeling of irradiation growth and thermal creep in zirconium cladding—Carlos Tome (MST-8)
- Neutron scattering applications to nuclear materials—Alice Smith (Nuclear Materials Science, MST-16)
- Computational modeling of long term kinetic processes in materials with atomistic insights—Donghua Xu (Oregon State University)
- Nuclear materials and fuels research at UF—Assel Aitkaliyeva (University of Florida)
- Multiscale modeling of radiation induced microstructural evolution and physical property degradation in materials—David Bai (Virginia Tech)

MST Division Leader David Teter (MST-DO) welcomed attendees and concluded the workshop, which included tours of the Ion Beam Materials Laboratory and the Electron Microscopy Laboratory in the Lab's Materials Science Complex. Laurent Capolungo (MST-8), Clarissa Yablinsky (MST-16), and Andy Nelson (MST-7) helped identify and

Nuclear scientist Alice Smith (MST-16), shown here using HIPPO, the high-pressure/preferred orientation diffractometer at the Los Alamos Neutron Science Center, discussed neutron scattering applications for nuclear materials at the workshop.

engage professors for the event. Esther Palluck (MST-8) prepared visitor agreements and Megan Espinoza (MST-8) and Angela Martinez (MST-8) controlled set-up and logistics over the course of the workshop.

Obrey said she has received positive feedback on the event, and new collaborations are forming as a result of this interaction. The Division has plans to maintain this momentum by hosting three more workshops on manufacturing science; damage, shock, and characterization; and polymer science.

The event was funded by the Momentum Initiative, which is owned by the Associate Directorate for Experimental Physical Sciences. The program sponsors the engagement of scientific communities to enhance Laboratory strategic partnerships, especially in the arena of mesoscale science.

Technical contact: Kim Obrey

Celebrating service

Congratulations to the following MST Division employees celebrating service anniversaries recently:

Bill Blumenthal, MST-8	35 years
Carl Cady, MST-8	30 years
Michael Torrez, MST-8	20 years
Dianne Wilburn, MST-DO	20 years
Kimberly Obrey, MST-8	15 years
Silas Romero, MST-16	15 years
Matthew Lee, MST-7	5 years
Nicholas Parra-Vasquez, MST-7	5 years

New technique breaks materials while collecting 3D x-ray images, improving understanding of materials' deformation and failure

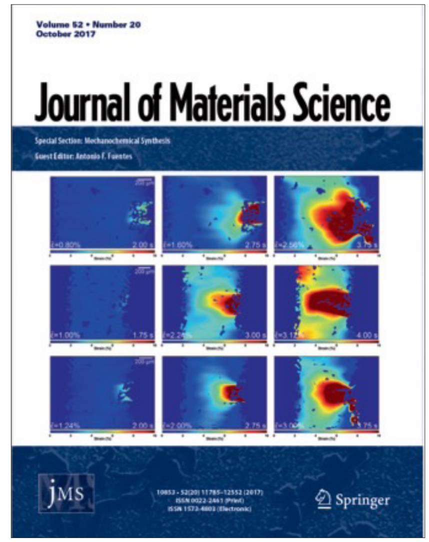
Engineered Materials (MST-7) researchers and colleagues developed a novel in situ x-ray tomographic imaging technique to break materials while collecting high-rate, three-dimensional images. This work, featured on the cover of *Journal of Materials Science*, collected 20 full three-dimensional (3D) x-ray images within 5 seconds using the x-ray beamline at Argonne National Laboratory's Advanced Photon Source, a success that could improve understanding of materials' deformation and failure.

The images were taken through a collaboration between Los Alamos, Arizona State University, and Argonne designed to investigate how advanced materials respond to uniaxial mechanical loading. Using x-ray computed microtomography and digital volume correlation, the team studied tensile behavior of an additively manufactured (AM) polymer matrix composite. The subject was a 3D-printed tensile dog bone made of a polymer-glass composite. The specimen was clamped within a mechanical load cell and pulled apart while the force response was measured. Simultaneously, the subject was rotated at 2 Hz within the synchrotron beam while researchers took thousands of x-ray radiographs that were then reconstructed to create a series of 3D images. Linking 3D images and load response allowed visualization of each of the processes that govern failure, including crack formation and propagation and the elastic response of the material. The role of print direction and recycled material upon the mechanical properties was also investigated. The study showed significant variations on strength and ductility from both vantages with respect to print direction and the recycled material content in the printed parts. The addition of recycled source material with a thermal history reduced the tensile strength of the AM composite for all directions, but the effect was drastic on the strength in the layering direction.

This capability is critical to understanding deformation and failure in materials in that the 3D imaging takes place while the material is being loaded. Current efforts in this multi-institutional collaboration have increased the imaging rate beyond the demonstrated 4-14 Hz. Future work will increase this 3D imaging upwards to 100 Hz, creating images critical to material model development and validation.

With MaRIE, the Lab's proposed experimental capability for studying matter-radiation interactions in extremes, researchers will be able to take this research further. MaRIE's combination of a unique hard x-ray free electron laser and in situ characterization tools would allow for measurements that are dynamic, in situ, and multi-modal. Such measurements are critical for capturing the sequential phenomena of composite mesoscale materials and could reveal properties that matter at the "middle" length scale that is often critical to controlling materials' performance.

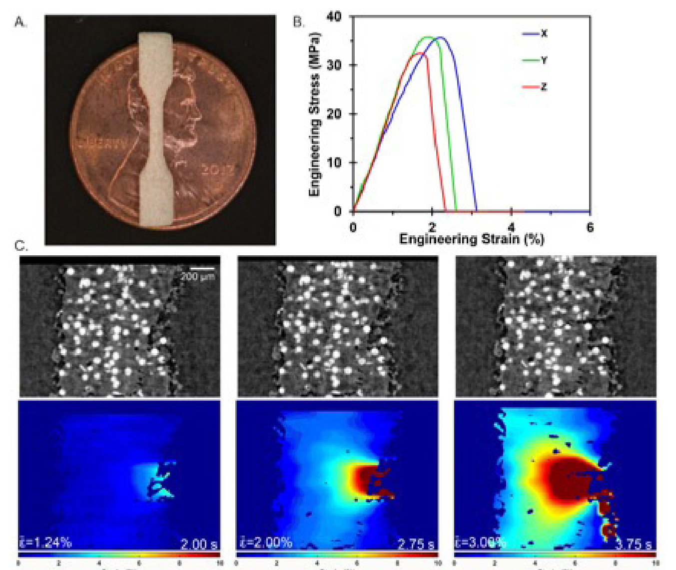
Capability development was supported by the Enhanced Surveillance Campaign (LANL Program Manager Tom Zocco), the Engineering Campaign (LANL Program Manager Antranik Siranosian), DSW (LANL Program Manager Jennifer Young), and Technology Maturation (LANL Program Manager Ryan Maupin). It supports the Lab's Stockpile Stewardship mission and its Materials of the Future science pillar.



Cover of the October 2017 *Journal of Materials Science*.

Researchers: James C.E. Mertens (formerly MST-7, now Intel); Brian M. Patterson, Kevin Henderson, and Nik Cordes (MST-7); Robin Pacheco (Sigma Division, Sigma-DO); Xianghui Xiao (Argonne National Laboratory); and Jason J. Williams and Nikhilesh Chawla (Arizona State University). Reference: "Analysis of thermal history effects on mechanical anisotropy of 3D-printed polymer matrix composites via in situ x-ray tomography," *Journal of Materials Science*, **52** (2017).

Technical contact: Brian M. Patterson



A) The 3D printed tensile specimen (dog-bone), stress strain curve during the tension experiment, and C) 3D reconstructed slices and digital volume correlation strain maps as a specimen pulls apart. Crack propagation is visible midway down the slices.

Study of damage in gallium-stabilized δ-plutonium stored at cryogenic temperatures

Predicting how radiation damage will alter the properties of a material and how those property changes evolve over time requires a detailed knowledge of the damage processes associated with radiation damage. Understanding the damaging effects of self-irradiation in plutonium (Pu) can be challenging, due in part to difficulties in obtaining appropriate potentials for Pu.

Plutonium metallurgy is inherently complex due to changes in chemistry and structure that result from radioactive decay. Simulations of the effects of self-irradiation of δ-Pu highlight the importance of the delicate interplay between damage creation processes and recovery processes in the evolution of microstructure. To separate those two processes and gain a better understanding of them, cryogenic aging can enable damaged local structure to accumulate quickly, followed by isochronal annealing to study the damage repair mechanisms as the material rewarms. The *Journal of Applied Physics* published these findings.

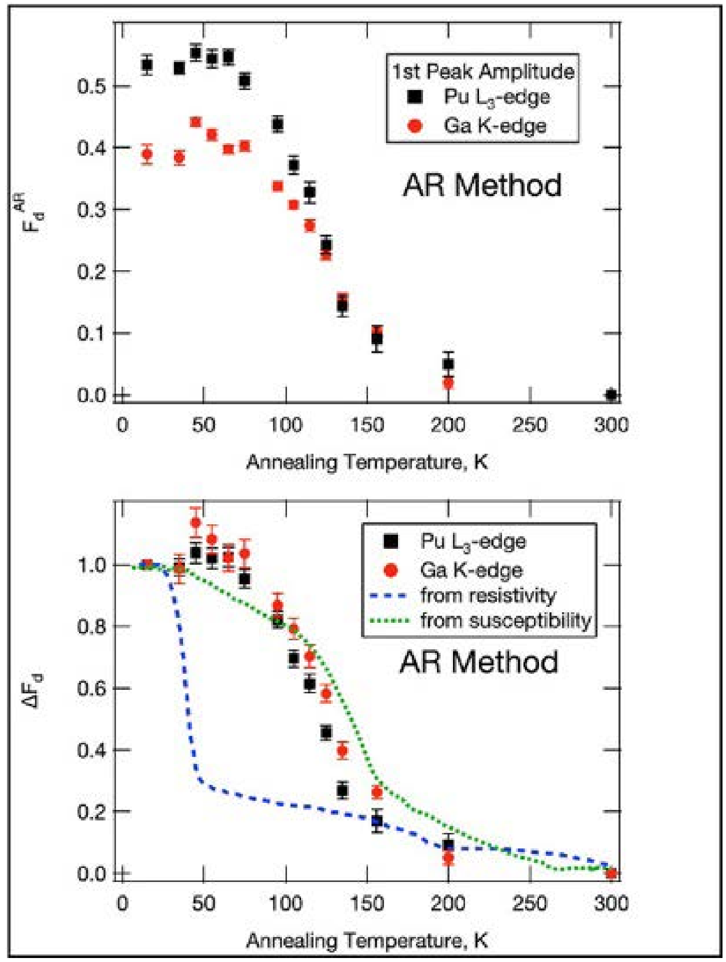
The team performed cryogenic aging to examine the damage creation and recovery processes in the evolution of Pu microstructure. They used extended x-ray absorption fine structure analysis to investigate self-irradiation damage on the local structure of gallium (Ga) stabilized δ-Pu stored at cryogenic temperatures. After 72 days of storage below 15 K, the investigators observed a loss of local order, indicating extensive damage. The effect occurred from both the Pu and the Ga sites, and shows changes in local coordination throughout the damage recovery process.

The team modeled the data using a spherical crystallite model to parameterize the size and fraction of undamaged regions in the material. This provided insight into damage production, annealing mechanisms, and the role of Ga in restoring order to the damaged lattice.

The primary practical interest in plutonium lies with its importance for energy generation applications in both nuclear power and nuclear weapons. However, there are also connections to fundamental science because understanding damage at the atomic level is complicated by plutonium's unique electronic and structural properties. An understanding of the electronic properties is required for calculating the structure and thermodynamics of plutonium and its compounds from first principles.

Reference: "Isochronal Annealing Effects on Local Structure, Crystalline Fraction, and Undamaged Region Size of Radiation Damage in Ga-stabilized δ-Pu," *Journal of Applied Physics* **120**, 035103 (2016).

Authors: Daniel T. Olive and Franz J. Freibert (Nuclear Materials Science, MST-16), Deborah L. Wang (Lawrence Berkeley National Laboratory and University of California – Berkeley), Corwin H. Booth, Scott K. McCall, Mark A. Wall, and Patrick G. Allen (Lawrence Berkeley National Laboratory); Eric D. Bauer (Condensed Matter and Magnet Science, MPA-CMMS), and Alison L. Pugmire (Engineered Materials, MST-7).



Top: Damage to local structure of δ-Pu after cold storage for 72 days below 15 K as determined by peak amplitude.

Bottom: The data are replotted to show the normalized fraction of residual damage present as a function of annealing temperature along with similarly normalized data from the previous resistivity and susceptibility isochronal annealing experiments.

The Laboratory Directed Research and Development program and the Glenn T. Seaborg Institute for Transactinium Science funded the work at Los Alamos. The research supports the Lab's Nuclear Deterrence and Energy Security missions and its Materials for the Future science pillar by providing insight into the effects of radiation damage on plutonium.

Technical contact: Dan Olive

Your soles will say thank you!

A new concrete walkway makes getting from the Materials Science Laboratory to the parking lot one smooth journey.

Los Alamos recognized as top diversity employer

For the second straight year, Los Alamos National Laboratory was recognized as a top diversity employer by *LATINA Style* and *STEM Workforce Diversity* magazine. Los Alamos rose in ranking to 10 on *STEM Workforce Diversity* magazine's Top Government Employers list and to 41 on *LATINA Style*'s Top 50 Companies list.

"We are pleased that the Laboratory is being recognized for its efforts to build a diverse and engaged workforce. This is an integral aspect of our staffing plans," said Carol Burns, deputy principal associate director for Science, Technology, and Engineering. "Diversity in our workforce gives us diversity in our perspective and thinking about the challenging problems inherent to our missions. It makes us more innovative."

On the list of Top 20 government employers, Los Alamos was named among agencies such as NASA and the National Institutes of Health. On *LATINA Style*'s Top 50 Companies, the Laboratory was named alongside the likes of AT&T, Hilton, and State Farm. Learn more at www.lanl.gov/discover/news-release-archive/2017/September/0919-top-diversity-employer.php.

Interesting in helping to shape the Lab workforce of the future?

The Lab's Employee Resource Groups were formed to help foster diversity and inclusion and to develop initiatives that assist the Lab in meeting its diversity-related goals and objectives. Active groups at the Lab include the following.

- American Indian,
- Disabilities Awareness,
- Lesbian, Gay, Bisexual, Transgender, and Intersex,
- Veterans, and
- Women.

If you are interested in volunteering on any of the above groups, please contact the Office of Diversity and Strategy Staffing at odss@lanl.gov.

HeadsUP!

Making room for new electron microscopy equipment

A concerted effort headed by members of the Materials Science and Technology Division led to the successful removal of a more than 20-year-old transmission electron microscope (TEM) from the Electron Microscopy Laboratory in the Materials Science Laboratory (MSL).

Two newer TEMs located in the MSL offer improved resolution and analytical capabilities over the outgoing JEOL 3000F TEM, which was chiefly used for atomic-scale microstructure characterization of materials. Removal activities ramped up with the arrival of an FEI Apreo, a scanning electron microscope that features a compound lens design and compatibility with a broad range of materials. The FEI Apreo will mainly be used for crystallographic and chemical characterization of material microstructures at the nanometer to millimeter scales.

Rodney McCabe (Materials Science in Radiation and Dynamics Extremes, MST-8), Roberta Beal (MST-8), Rafael Spillers (Nuclear Materials Science, MST-16), and Cody Miller (Sigma Division, Sigma-DO) logged several hours facilitating the equipment's removal—detaching equipment, unplugging cables, and removing vacuum components. During the removal process, the Lab's Chief Electrical Safety Officer Lloyd Gordon (Industrial Safety and Hygiene, OSH-ISH) verified that the instrument was in an electrically safe state and that the equipment could not reenergize. Workers, led by Levi Masingale (Logistics Superintendent Field Work Execution, LOG-SUP), did the literal heavy lifting, using a crane to remove large pieces of the microscope. Once safely secured in a truck, the JEOL 3000F was moved to Warehousing and Salvage Operations to be used for spare parts as needed.

This effort supports the "Clean the Past" objective of the Experimental Physical Sciences Directorates Environmental Action Plan. Other MST housekeeping days held earlier this year led to the removal of assorted furniture, office supplies, electronics, unneeded equipment, and dozens of burn boxes. Housekeeping days are designed to improve safety and operational efficiency across the Lab. MST-specific efforts were led by Rafael Spillers (MST-16); Roberta Beal, Saryu Fensin, Ted Holby, Michael Torrez, Ramon Martinez, and Dominic Roybal (MST-8); Andres Villanueva (Science and Technology Operations, MSS-STO); and Nix Mattson (Property Management, ASM-PM).

Technical contact: Roberta Beal

The JEOL 3000 was removed in three large pieces and several smaller pieces. Above, riggers stabilize the microscope's high tension tank on a dolly. To the left of the riggers is the microscope frame that housed the tank, the TEM column, and other components. Below, the TEM column on a dolly outside the Materials Science Laboratory.

MST e-NEWS

Published by the Experimental Physical Sciences Directorate.

To submit news items or for more information, contact Karen Kippen, ADEPS Communications, at 505-606-1822, or adeps-comm@lanl.gov.

For past issues, see www.lanl.gov/org/padste/adeps/mst-e-news.php.

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